Electronic Supplementary Information

Energetic Derivatives Substituted with Trinitrophenyl: Improving the Sensitivity of Explosives

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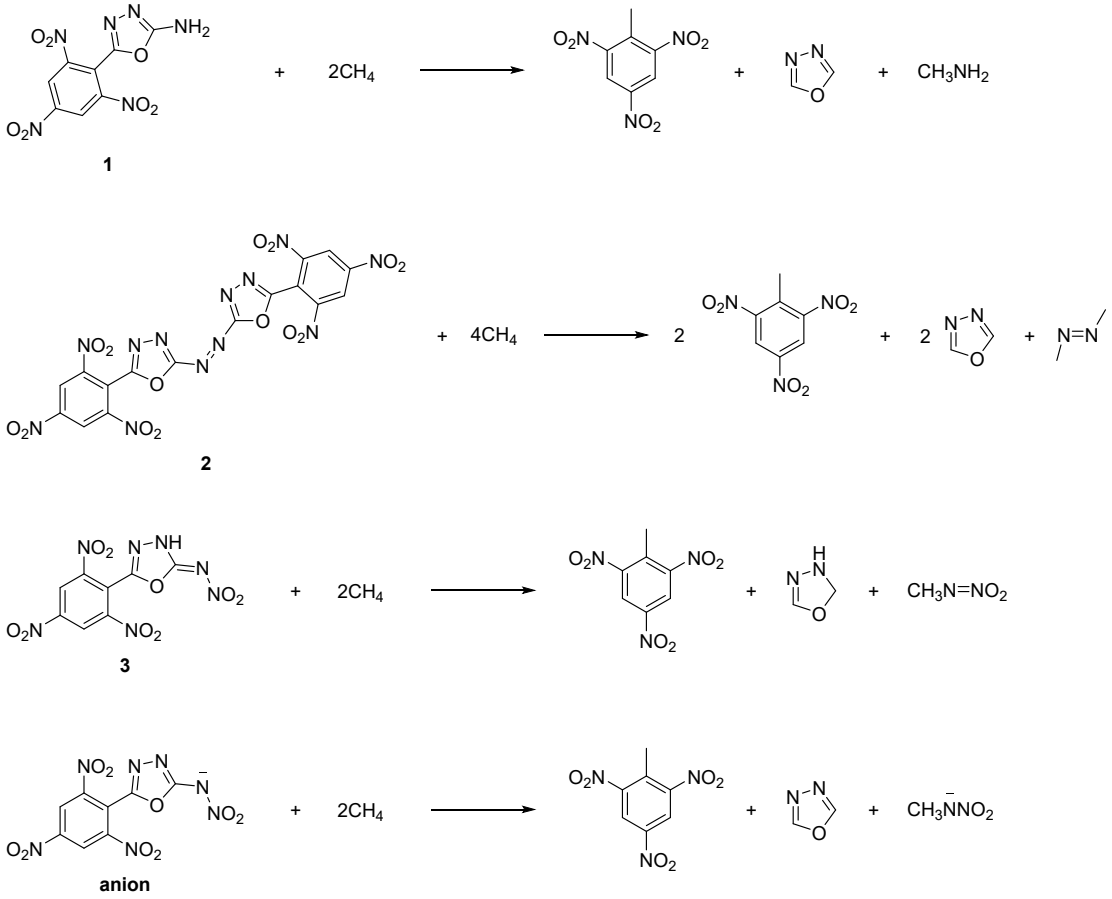
Theoretical Calculations

The structures of compounds **1**, **2**, **3**, **4**, **6a** and **6b** were optimized at the M062X/def2tzvp level to obtain their stable structures on the potential energy surface, using the Gaussian 16A program.[1] After vibration analysis, there were no imaginary frequencies. In order to obtain the heat of gas phase formation of the compounds, their isodesmic reactions were reasonably designed (**Scheme S1**).



Scheme S1. Isodesmic reactions for the heats of formation.

Using the atomization method, the gas phase enthalpy of the constructed model molecule was calculated using the G3 ab initio algorithm.[2]

Table S1. The heats of formation (HOF) for **1**, **2**, **3** and **anion**[a].

Compounds	**ZPE[b] (Hartree/Particle)**	**H_T [c] (Hartree/Particle)**	**M062X/def2tzvp (Hartree/Particle)**	**HOF(gas) (kJ mol^{-1})**
CH_4	0.045026	0.048836	-40.5002716	-74.9[d]
CH_3NH_2	0.064218	0.068552	-95.8424359	-23.5[d]
CH_2=NNO_2	0.067592	0.073707	-300.3457738	2.2
$CH_3N^-NO_2$	0.053614	0.059231	-299.7881826	-99.4
1	0.150827	0.018174	-1162.0201282	155.0489054
2	0.256589	0.034995	-2321.5527447	666.5629524
3	0.153523	0.020265	-1366.500766	222.6463686
anion	0.139638	0.02024	-1365.9961683	0.174175772

[a] The enthalpy of sublimation was calculated by using Trouton's rule. The solid-state heats of formation of the resulting compounds were calculated with Equation (1) in which Tm is the melting temperature. $\Delta H_f = \Delta H_f(g) - \Delta H_{sub} = \Delta H_f(g) - 188[J\ mol^{-1}\ K^{-1}] \times T_m$ (1). [b] Zero-point correction. [c] Thermal correction to enthalpy, i.e., $H_{298.15\ K} - H_{0\ K}$.[d] NIST WebBook.

Crystallographic Data

Table S2. Crystallographic data for compounds 2 and 3.

Compound	**2**	**3**
CCDC number	2286868	2133005
Formula	$C_{26}H_{24}N_{12}O_{19}$	$C_8H_3N_7O_9$
$D_{calc.}$/ g cm^{-3}	1.576	1.865
μ/mm^{-1}	0.137	1.537
Formula Weight	808.57	341.17
Colour	pale yellow	colourless
Shape	plate	plate
Size/mm^3	0.07×0.12×0.13	0.06×0.05×0.02
T/K	301.0	100.00(10)
Crystal System	triclinic	orthorhombic
Space Group	*P-1*	*Pbca*
a/Å	8.217(2)	12.0361(2)
b/Å	9.115(2)	9.5416(2)
c/Å	12.762(4)	21.1634(4)
α/°	87.690(9)	90
β/°	75.875(9)	90
γ/°	67.078(6)	90
V/Å^3	852.1(4)	2430.49(9)
Z	1	8
Z'	0.5	1
Wavelength/Å	0.71073	1.54184
Radiation type	MoK_α	$Cu\ K_\alpha$
Θ_{min}/°	2.17	4.178
Θ_{max}/°	26.11	77.144
Measured Refl's.	31063	13994
Indep't Refl's	3699	2520
R_{int}	0.0883	0.0374
Parameters	298	221
Restraints	0	0
Largest Peak	0.731	0.204
Deepest Hole	-0.346	-0.268
GooF	1.035	1.073
wR_2 **(all data)**	0.1770	0.0767
wR_2	0.1527	0.0746
R_1 **(all data)**	0.0877	0.0346
R_1	0.0579	0.0306

Table S3: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
O1	3902.4(8)	4217.4(9)	4869.5(4)	15.0(2)
O2	2951.3(8)	6460.1(10)	6613.5(4)	16.9(2)
O3	2863.0(8)	4182.9(10)	6637.1(4)	17.9(2)
O4	5415.6(8)	1719.0(11)	4855.1(4)	20.8(2)
O5	5972.9(8)	117.6(10)	4197.5(5)	21.2(2)
O6	5771.4(11)	1149.2(13)	1986.1(5)	35.4(3)
O7	4734.0(9)	2860.9(11)	1666.5(5)	23.9(2)
O8	1858.9(9)	4505.4(12)	3032.3(5)	29.5(3)
O9	2096.4(9)	4490.6(12)	4042.9(5)	27.4(3)
N1	2984.7(9)	2953.0(12)	5531.0(5)	14.2(2)
N2	3008.5(9)	2185.2(11)	4972.7(5)	15.0(2)
N3	3627.4(9)	5333.3(11)	5800.2(5)	15.1(2)
N4	3126.1(9)	5289.1(11)	6371.9(5)	13.4(2)
N5	5440.4(9)	1168.4(12)	4332.8(5)	15.2(2)
N6	5074.5(10)	2065.0(12)	2072.6(5)	18.5(2)
N7	2357.8(9)	4151.1(12)	3507.8(5)	16.7(2)
C1	3495.6(10)	4174.1(13)	5461.7(6)	13.4(2)
C2	3561.3(10)	2977.9(13)	4603.4(6)	13.2(2)
C3	3902.0(10)	2694.4(13)	3944.9(6)	13.3(2)
C4	4809.7(10)	1831.9(13)	3814.2(6)	13.1(2)
C5	5188.5(10)	1579.4(13)	3208.0(6)	14.4(3)
C6	4635.8(11)	2230.3(13)	2719.1(6)	14.4(3)
C7	3700.5(11)	3049.9(13)	2806.6(6)	15.1(3)
C8	3351.7(10)	3256.0(13)	3422.0(6)	14.2(3)

Table S4: Anisotropic Displacement Parameters ($\times 10^4$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	18.3(4)	15.0(4)	11.7(4)	-1.4(3)	2.0(3)	-2.1(3)
O2	21.5(5)	13.7(4)	15.6(5)	-3.0(4)	0.6(3)	1.2(4)
O3	25.4(5)	14.3(5)	14.0(4)	1.9(3)	2.1(4)	-2.5(4)
O4	20.7(5)	30.0(5)	11.8(5)	-0.8(4)	-1.1(3)	2.3(4)
O5	21.9(5)	19.1(5)	22.5(5)	3.0(4)	0.5(4)	7.0(4)
O6	49.9(7)	35.2(6)	20.9(5)	0.7(5)	11.6(5)	23.5(6)
O7	25.5(5)	31.6(6)	14.5(5)	6.7(4)	1.3(4)	3.3(4)
O8	28.0(5)	43.0(7)	17.5(5)	4.9(4)	-2.1(4)	17.8(5)
O9	30.6(6)	35.4(6)	16.1(5)	-2.9(4)	1.7(4)	16.2(5)
N1	18.0(5)	14.5(5)	10.2(5)	-0.9(4)	1.6(4)	-0.4(4)
N2	17.4(5)	16.2(5)	11.4(5)	-1.5(4)	0.5(4)	1.2(4)

N3	17.4(5)	15.8(5)	12.0(5)	-1.0(4)	2.4(4)	-1.1(4)
N4	14.0(5)	14.4(5)	11.9(5)	0.0(4)	-1.3(4)	-0.5(4)
N5	13.3(5)	17.3(5)	15.0(5)	2.9(4)	0.2(4)	-0.4(4)
N6	21.4(6)	20.2(6)	13.8(5)	-1.1(4)	1.6(4)	0.3(4)
N7	17.2(5)	17.5(6)	15.4(5)	2.2(4)	0.5(4)	2.7(4)
C1	13.1(5)	15.7(6)	11.4(6)	1.5(5)	0.6(4)	1.1(5)
C2	13.5(6)	12.5(6)	13.5(6)	-1.0(5)	-1.2(4)	1.3(4)
C3	14.7(6)	12.6(6)	12.7(6)	-0.6(5)	0.3(4)	-2.8(5)
C4	14.0(6)	12.6(6)	12.7(6)	1.4(5)	-2.2(4)	-1.5(4)
C5	13.9(6)	13.0(6)	16.3(6)	-0.7(5)	0.3(5)	-1.0(5)
C6	17.4(6)	13.6(6)	12.4(6)	-2.1(5)	2.0(5)	-2.3(5)
C7	17.0(6)	14.2(6)	14.3(6)	1.4(5)	-1.6(5)	-1.7(5)
C8	14.6(6)	12.4(6)	15.6(6)	0.3(5)	0.1(5)	0.3(5)

Table S5: Bond Lengths in Å for **2**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C1	1.349(3)	C10	C16	1.373(3)
O1	C6	1.355(3)	C12	C14	1.389(3)
N1	N1	1.256(4)	C12	C16	1.379(3)
N1	C6	1.387(3)	C2	C9	1.440(5)
O4	N4	1.220(3)	C9	C2	1.440(5)
O6	N4	1.211(3)	O2	C5	1.461(17)
N4	C10	1.471(3)	O2	C11	1.46(2)
O8	C2	1.418(4)	O2	C13	1.54(2)
O8	C9	1.406(4)	O2	C7	1.58(2)
O10	N6	1.204(3)	C5	C11	1.505(13)
N6	O3	1.204(3)	C5	C7	1.223(11)
N6	C8	1.478(3)	C5	O5	1.56(2)
N3	O11	1.203(3)	C11	C5	1.505(13)
N3	O7	1.204(3)	C11	C13	1.231(12)
N3	C12	1.470(3)	C11	O5	1.60(2)
N2	N5	1.399(3)	O9	C3	1.416(11)
N2	C1	1.277(3)	O9	C15	1.446(12)
N5	C6	1.281(3)	C3	C7	1.508(12)
C1	C14	1.481(3)	C13	C15	1.477(13)
C4	C8	1.376(3)	C13	O5	1.40(2)
C4	C10	1.372(3)	C7	O5	1.39(2)
C8	C14	1.391(3)			

Table S6: Bond Angles in ° for **2**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C1	O1	C6	101.09(18)	C5	O2	C7	47.3(6)
N1	N1	C6	112.9(2)	C11	O2	C13	48.4(7)
O4	N4	C10	117.5(2)	C11	O2	C7	114.3(10)
O6	N4	O4	124.9(2)	C13	O2	C7	96.1(12)
O6	N4	C10	117.6(2)	O2	C5	C11	111.8(11)
C9	O8	C2	110.5(3)	O2	C5	O5	13.0(16)
O10	N6	O3	124.5(2)	C11	C5	O5	124.5(10)

O10	N6	C8	117.4(2)	C7	C5	O2	71.4(11)
O3	N6	C8	118.0(2)	C7	C5	C11	168.7(9)
O11	N3	O7	123.7(2)	C7	C5	O5	58.4(10)
O11	N3	C12	117.9(2)	O2	C11	C5	112.2(11)
O7	N3	C12	118.4(2)	O2	C11	O5	12.3(16)
C1	N2	N5	105.7(2)	C5	C11	O5	123.9(10)
C6	N5	N2	105.5(2)	C13	C11	O2	68.8(10)
O1	C1	C14	119.4(2)	C13	C11	C5	176.3(9)
N2	C1	O1	114.0(2)	C13	C11	O5	57.4(10)
N2	C1	C14	126.6(2)	C3	O9	C15	110.5(6)
C10	C4	C8	116.7(2)	O9	C3	C7	110.7(7)
O1	C6	N1	122.3(2)	C11	C13	O2	62.8(9)
N5	C6	O1	113.7(2)	C11	C13	C15	161.3(9)
N5	C6	N1	124.0(2)	C11	C13	O5	74.8(11)
C4	C8	N6	116.5(2)	C15	C13	O2	124.6(11)
C4	C8	C14	123.9(2)	O5	C13	O2	12.9(17)
C14	C8	N6	119.6(2)	O5	C13	C15	111.7(12)
C4	C10	N4	119.2(2)	C5	C7	O2	61.3(9)
C4	C10	C16	123.1(2)	C5	C7	C3	172.2(8)
C16	C10	N4	117.7(2)	C5	C7	O5	73.0(11)
C14	C12	N3	120.6(2)	C3	C7	O2	124.8(10)
C16	C12	N3	116.6(2)	O5	C7	O2	11.7(16)
C16	C12	C14	122.8(2)	O5	C7	C3	113.2(12)
C8	C14	C1	121.3(2)	O9	C15	C13	111.1(7)
C12	C14	C1	122.9(2)	C5	O5	C11	93.9(12)
C12	C14	C8	115.7(2)	C13	O5	C5	128.4(14)
C10	C16	C12	117.7(2)	C13	O5	C11	47.8(9)
O8	C2	C9	113.5(3)	C7	O5	C5	48.6(8)
O8	C9	C2	112.5(3)	C7	O5	C11	117.3(13)
C5	O2	C11	104.4(9)	C7	O5	C13	112.3(15)
C5	O2	C13	125.6(11)				

Table S7: Torsion Angles in ° for **2**

Atom	**Atom**	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	C1	C14	C8	-97.0(3)	C5	O2	C11	C13	-125.1(14)
O1	C1	C14	C12	86.5(3)	C5	O2	C11	O5	-105(5)
N1	N1	C6	O1	1.2(4)	C5	O2	C13	C11	76.9(17)
N1	N1	C6	N5	-179.2(3)	C5	O2	C13	C15	-83.0(19)
O4	N4	C10	C4	-21.8(3)	C5	O2	C13	O5	-81(5)
O4	N4	C10	C16	157.8(2)	C5	O2	C7	C3	174.3(11)
O6	N4	C10	C4	158.7(2)	C5	O2	C7	O5	-180(8)

O6	N4	C10	C16	-21.7(3)	C5	C11	O5	C5	43.1(15)
N4	C10	C16	C12	179.9(2)	C5	C11	O5	C13	-175.8(11)
O10	N6	C8	C4	28.3(3)	C5	C11	O5	C7	87.9(18)
O10	N6	C8	C14	-152.2(3)	C5	C7	O5	C11	-69.5(15)
N6	C8	C14	C1	4.0(3)	C5	C7	O5	C13	-122.2(17)
N6	C8	C14	C12	-179.3(2)	C11	O2	C5	C11	-58.5(15)
N3	C12	C14	C1	-3.5(4)	C11	O2	C5	C7	109.9(13)
N3	C12	C14	C8	179.8(2)	C11	O2	C5	O5	110(7)
N3	C12	C16	C10	-179.7(2)	C11	O2	C13	C15	-159.9(11)
O11	N3	C12	C14	174.0(3)	C11	O2	C13	O5	-158(5)
O11	N3	C12	C16	-7.3(4)	C11	O2	C7	C5	-87.4(13)
N2	N5	C6	O1	-0.3(3)	C11	O2	C7	C3	86.9(14)
N2	N5	C6	N1	-179.9(2)	C11	O2	C7	O5	93(8)
N2	C1	C14	C8	82.6(3)	C11	C5	C7	O2	108(4)
N2	C1	C14	C12	-94.0(3)	C11	C5	C7	O5	108(4)
O3	N6	C8	C4	-153.4(3)	C11	C5	O5	C11	-43.5(15)
O3	N6	C8	C14	26.1(4)	C11	C5	O5	C13	-80(2)
N5	N2	C1	O1	-0.6(3)	C11	C5	O5	C7	-167.0(11)
N5	N2	C1	C14	179.8(2)	C11	C13	C15	O9	-51(3)
C1	O1	C6	N1	179.6(2)	C11	C13	O5	C5	53.1(19)
C1	O1	C6	N5	-0.1(3)	C11	C13	O5	C7	107.2(16)
C1	N2	N5	C6	0.5(3)	O9	C3	C7	O2	-51.6(13)
O7	N3	C12	C14	-5.8(4)	O9	C3	C7	O5	-52.9(13)
O7	N3	C12	C16	172.9(3)	C3	O9	C15	C13	-56.3(8)
C4	C8	C14	C1	-176.7(2)	C3	C7	O5	C5	175.0(10)
C4	C8	C14	C12	0.1(3)	C3	C7	O5	C11	105.5(16)
C4	C10	C16	C12	-0.6(4)	C3	C7	O5	C13	52.7(18)
C6	O1	C1	N2	0.5(3)	C13	O2	C5	C11	-107.3(18)
C6	O1	C1	C14	-179.9(2)	C13	O2	C5	C7	61.2(17)
C8	C4	C10	N4	-178.7(2)	C13	O2	C5	O5	61(6)
C8	C4	C10	C16	1.7(4)	C13	O2	C11	C5	-176.1(10)
C10	C4	C8	N6	177.9(2)	C13	O2	C11	O5	20(5)
C10	C4	C8	C14	-1.5(4)	C13	O2	C7	C5	-134.2(11)
C14	C12	C16	C10	-1.0(4)	C13	O2	C7	C3	40.1(13)
C16	C12	C14	C1	177.9(2)	C13	O2	C7	O5	46(7)
C16	C12	C14	C8	1.2(3)	C13	C11	O5	C5	-141.1(13)
C2	O8	C9	C2	-52.0(5)	C13	C11	O5	C7	-96.3(18)
C9	O8	C2	C9	52.6(5)	C7	O2	C5	C11	-168.4(9)
O2	C5	C7	O5	0.0(16)	C7	O2	C5	O5	0(6)
O2	C5	O5	C11	-56(6)	C7	O2	C11	C5	108.1(13)
O2	C5	O5	C13	-93(7)	C7	O2	C11	C13	-75.8(14)
O2	C5	O5	C7	-180(7)	C7	O2	C11	O5	-56(5)
O2	C11	C13	C15	118(3)	C7	O2	C13	C11	117.3(9)
O2	C11	C13	O5	5.0(13)	C7	O2	C13	C15	-42.6(11)
O2	C11	O5	C5	62(5)	C7	O2	C13	O5	-40(5)
O2	C11	O5	C13	-157(6)	C7	C5	O5	C11	123.4(13)
O2	C11	O5	C7	106(6)	C7	C5	O5	C13	87(2)
O2	C13	C15	O9	56.6(11)	C15	O9	C3	C7	53.7(8)
O2	C13	O5	C5	74(5)	C15	C13	O5	C5	-108(2)
O2	C13	O5	C11	20(5)	C15	C13	O5	C11	-161.5(10)
O2	C13	O5	C7	128(6)	C15	C13	O5	C7	-54.3(18)
O2	C7	O5	C5	0(7)	O5	C5	C7	O2	0.0(16)
O2	C7	O5	C11	-69(7)	O5	C11	C13	O2	-5.0(13)
O2	C7	O5	C13	-122(8)	O5	C11	C13	C15	113(3)

C5	O2	C11	C5	58.8(15)	O5	C13	C15	O9	56.0(12)

Table S8: Bond Lengths in Å for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.3460(15)	N3	N4	1.3527(15)
O1	C2	1.3727(15)	N3	C1	1.3274(17)
O2	N4	1.2466(14)	N5	C4	1.4770(16)
O3	N4	1.2367(14)	N6	C6	1.4750(16)
O4	N5	1.2242(15)	N7	C8	1.4810(16)
O5	N5	1.2239(15)	C2	C3	1.4778(17)
O6	N6	1.2250(16)	C3	C4	1.3954(18)
O7	N6	1.2179(15)	C3	C8	1.3966(18)
O8	N7	1.2196(15)	C4	C5	1.3828(18)
O9	N7	1.2192(15)	C5	C6	1.3780(18)
N1	N2	1.3905(15)	C6	C7	1.3832(18)
N1	C1	1.3256(17)	C7	C8	1.3823(18)
N2	C2	1.2750(17)			

Table S9: Bond Angles in ° for **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C2	104.28(10)	N3	C1	O1	115.69(11)
C1	N1	N2	111.07(10)	O1	C2	C3	117.49(11)
C2	N2	N1	102.65(10)	N2	C2	O1	114.57(11)
C1	N3	N4	113.80(10)	N2	C2	C3	127.90(12)
O2	N4	N3	114.47(10)	C4	C3	C2	120.80(11)
O3	N4	O2	122.39(10)	C4	C3	C8	116.14(11)
O3	N4	N3	123.15(11)	C8	C3	C2	123.06(11)
O4	N5	C4	118.32(11)	C3	C4	N5	120.53(11)
O5	N5	O4	125.14(11)	C5	C4	N5	116.44(11)
O5	N5	C4	116.51(11)	C5	C4	C3	123.01(12)
O6	N6	C6	117.38(11)	C6	C5	C4	117.32(12)
O7	N6	O6	124.74(12)	C5	C6	N6	118.39(11)
O7	N6	C6	117.87(11)	C7	C6	N6	118.43(11)
O8	N7	O9	124.45(11)	C7	C6	C5	123.17(12)
O8	N7	C8	117.15(11)	C6	C7	C8	116.99(12)
O9	N7	C8	118.40(11)	C3	C8	N7	120.47(11)
N1	C1	O1	107.39(11)	C7	C8	N7	116.29(11)
N1	C1	N3	136.73(12)	C7	C8	C3	123.22(12)

Table S10: Torsion Angles in ° for **3**

Atom	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Atom	Angle/°
O1	C2	C3	C4	98.97(14)	N6	C6	C7	C8	-176.03(11)
O1	C2	C3	C8	-81.06(15)	C1	O1	C2	N2	98.97(14)
O4	N5	C4	C3	-24.13(17)	C1	O1	C2	C3	-81.06(15)
O4	N5	C4	C5	154.14(12)	C1	N1	N2	C2	-24.13(17)

O5	N5	C4	C3	157.61(11)	C1	N3	N4	O2	154.14(12)
O5	N5	C4	C5	-24.12(16)	C1	N3	N4	O3	157.61(11)
O6	N6	C6	C5	13.80(18)	C2	O1	C1	N1	-24.12(16)
O6	N6	C6	C7	-167.25(13)	C2	O1	C1	N3	13.80(18)
O7	N6	C6	C5	-164.97(12)	C2	C3	C4	N5	-167.25(13)
O7	N6	C6	C7	13.98(18)	C2	C3	C4	C5	-164.97(12)
O8	N7	C8	C3	-173.66(12)	C2	C3	C8	N7	13.98(18)
O8	N7	C8	C7	7.78(17)	C2	C3	C8	C7	-173.66(12)
O9	N7	C8	C3	6.77(18)	C3	C4	C5	C6	7.78(17)
O9	N7	C8	C7	-171.80(12)	C4	C3	C8	N7	6.77(18)
N1	N2	C2	O1	-0.38(14)	C4	C3	C8	C7	-171.80(12)
N1	N2	C2	C3	177.21(12)	C4	C5	C6	N6	-0.38(14)
N2	N1	C1	O1	-2.34(14)	C4	C5	C6	C7	177.21(12)
N2	N1	C1	N3	172.03(14)	C5	C6	C7	C8	-2.34(14)
N2	C2	C3	C4	-78.56(17)	C6	C7	C8	N7	172.03(14)
N2	C2	C3	C8	101.41(17)	C6	C7	C8	C3	-78.56(17)
N4	N3	C1	O1	174.71(10)	C8	C3	C4	N5	101.41(17)
N4	N3	C1	N1	0.7(2)	C8	C3	C4	C5	174.71(10)
N5	C4	C5	C6	-177.70(11)					

NMR and IR spectra and DSC plots of 2-6

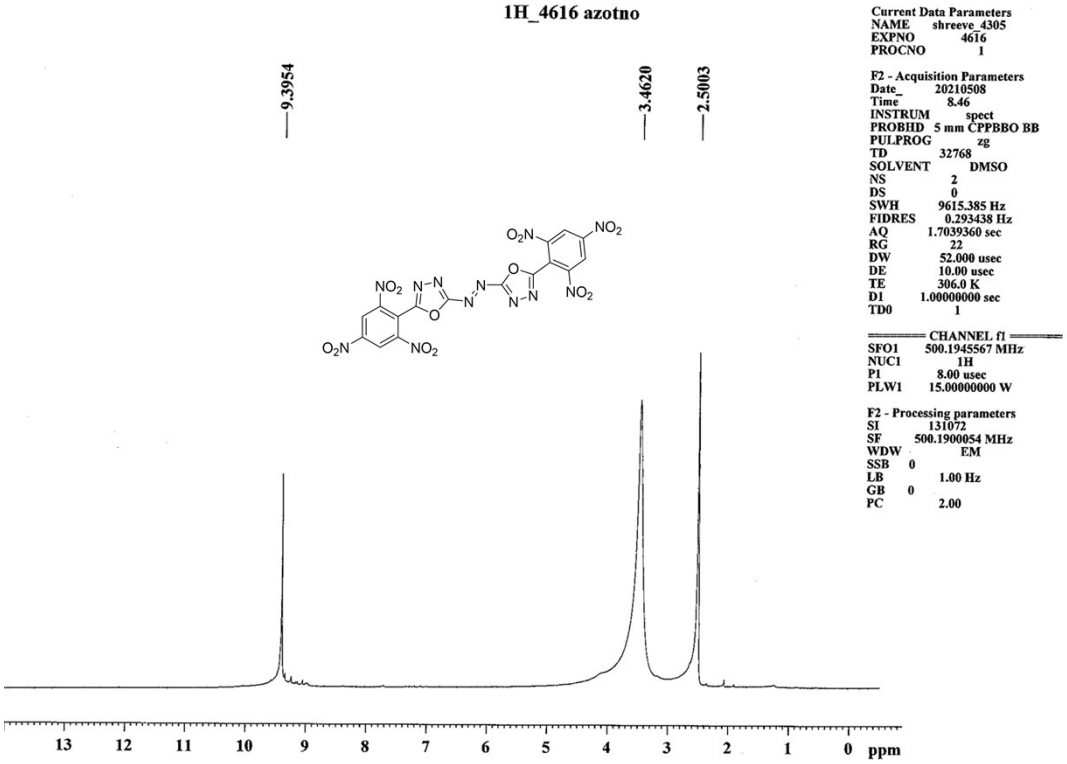


Figure S1 ^{1}H-NMR spectrum of **2** in d_6-DMSO.

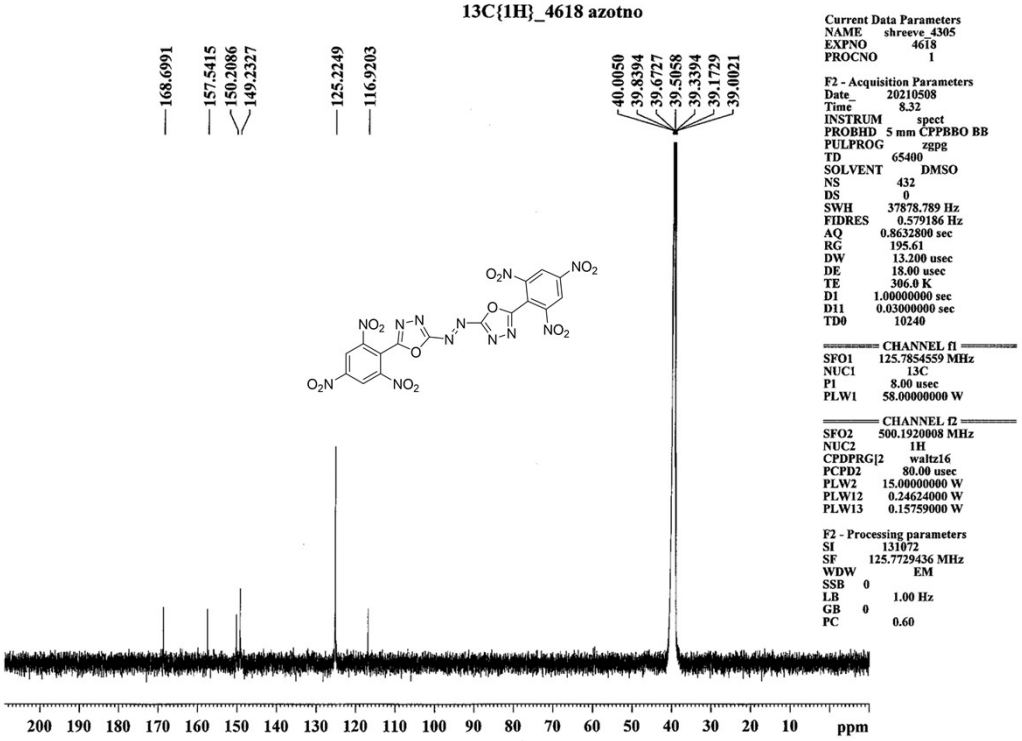


Figure S2 ^{13}C-NMR spectrum of **2** in d_6-DMSO.

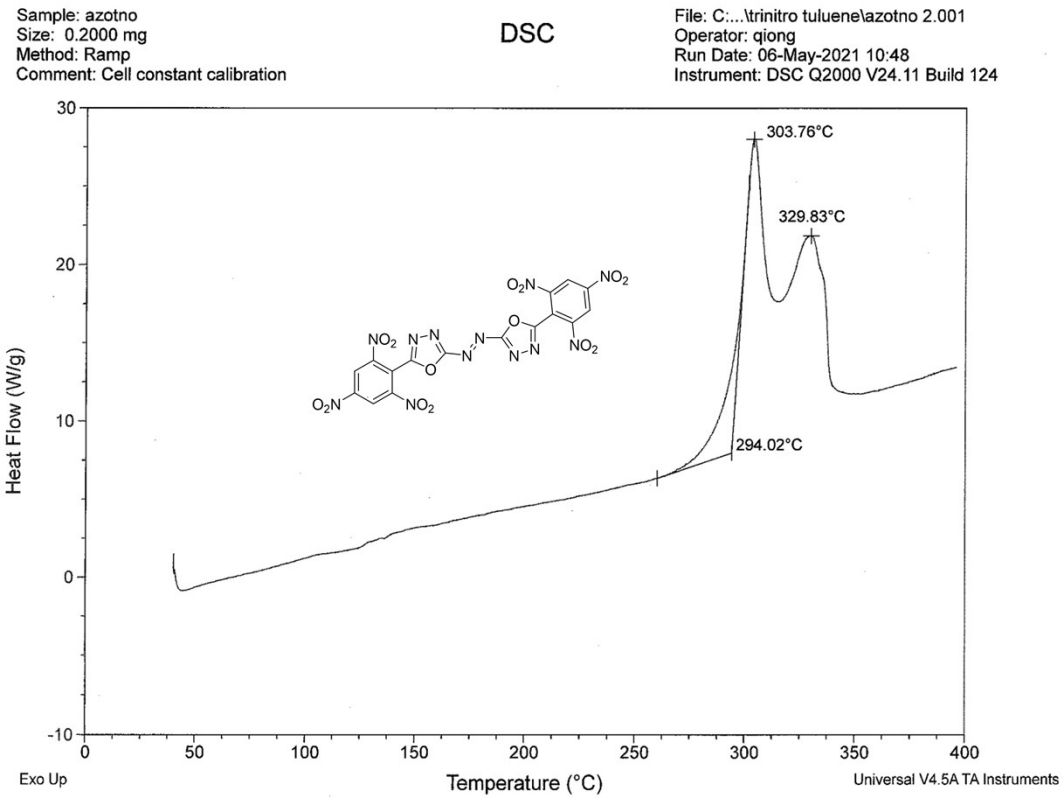


Figure S3 DSC plot of **2**.

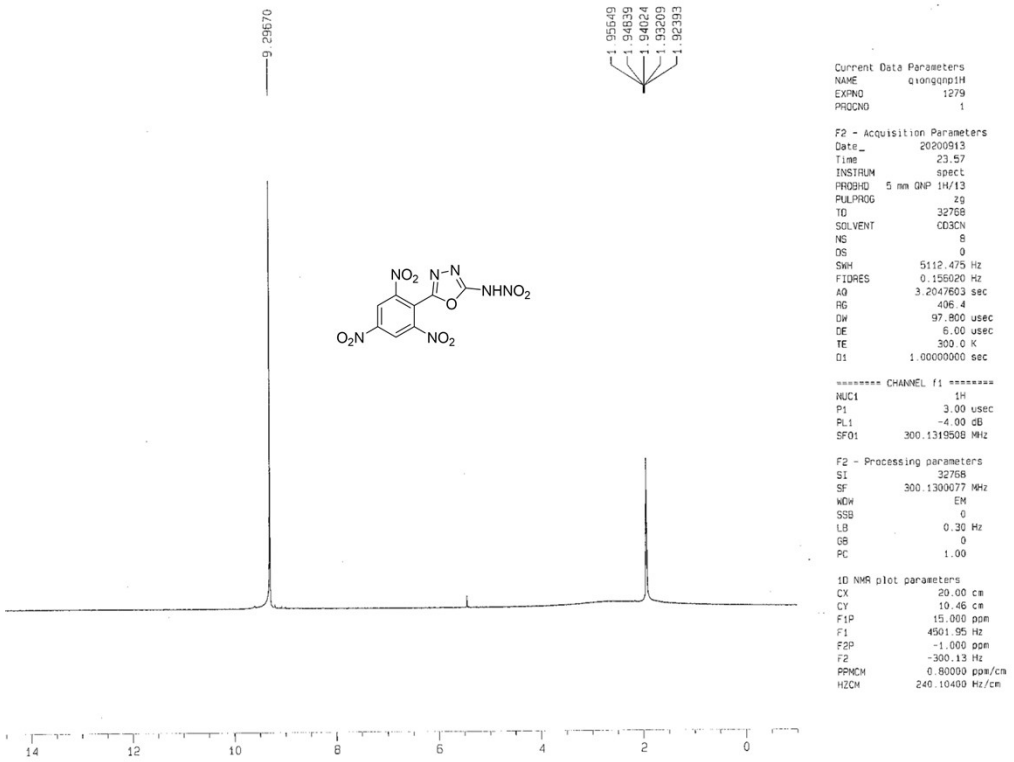


Figure S4 ^{1}H-NMR spectrum of **3** in CD_3CN.

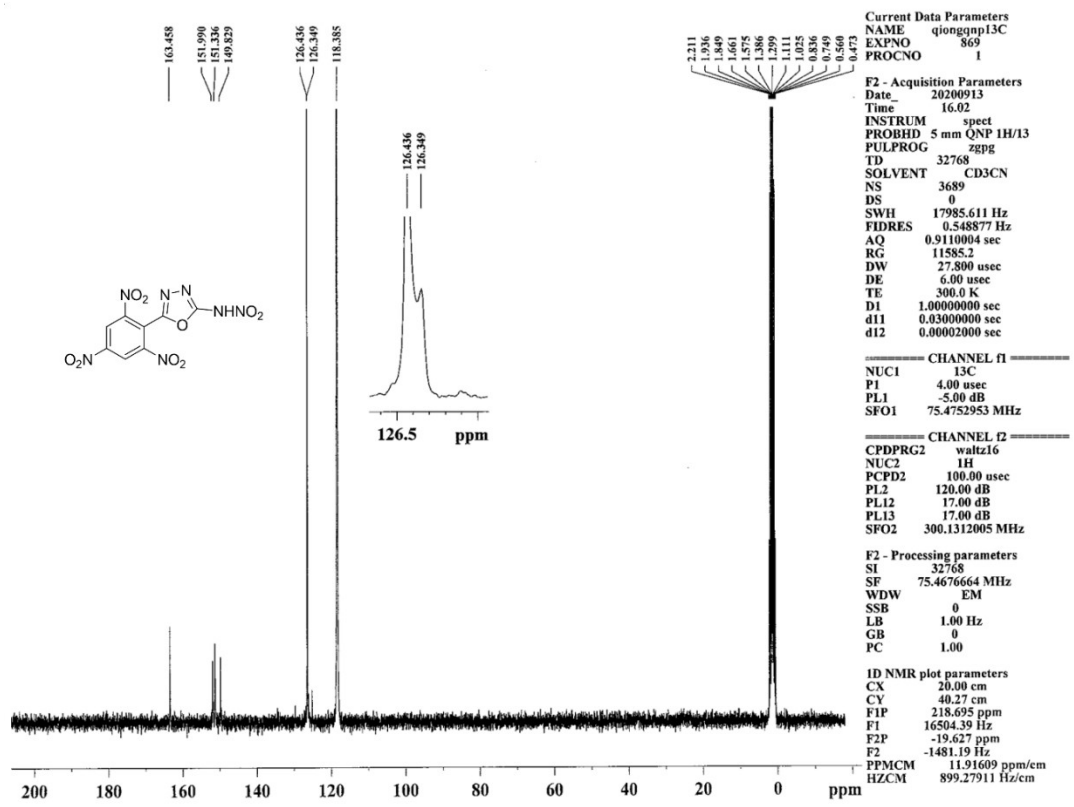


Figure S5 ^{13}C-NMR spectrum of **3** in CD_3CN.

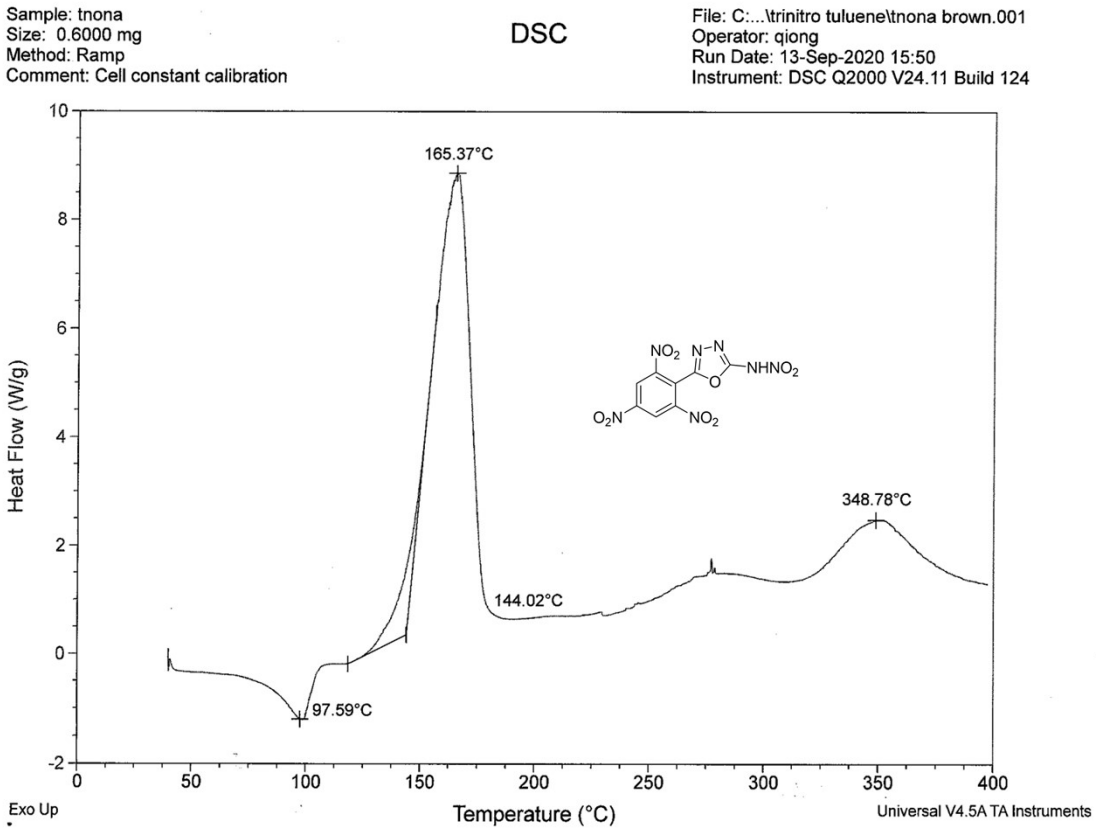


Figure S6 DSC plot of **3**.

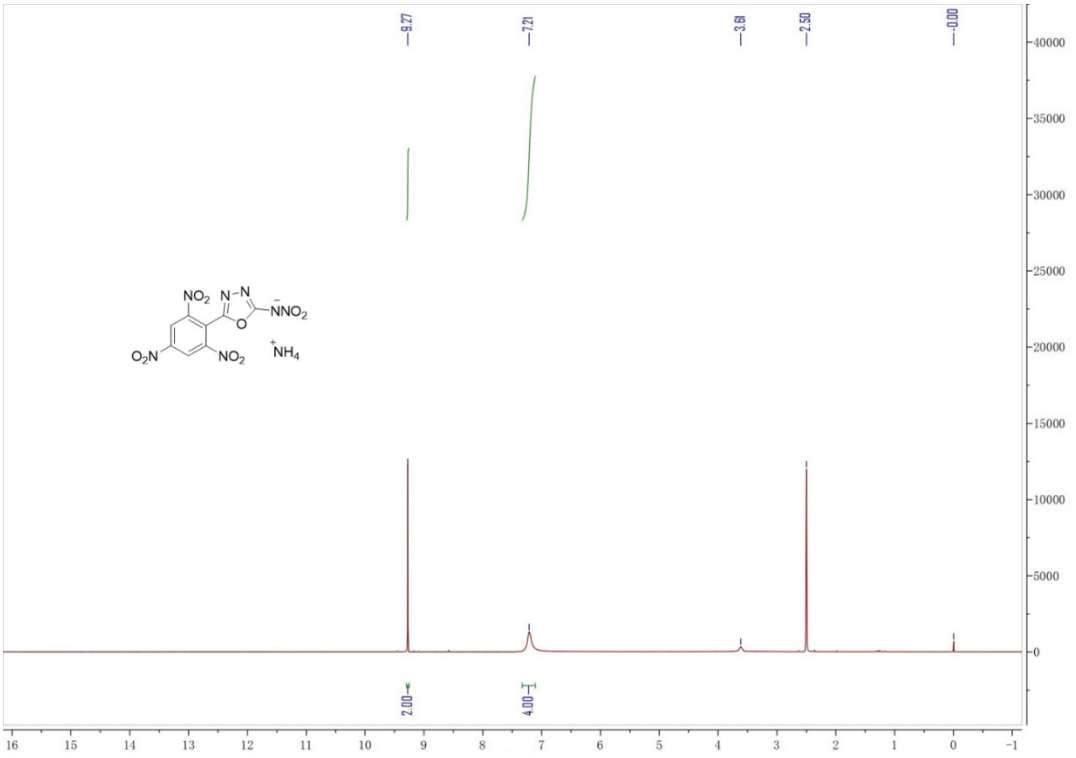


Figure S7 ^{1}H-NMR spectrum of **4** in d_6-DMSO.

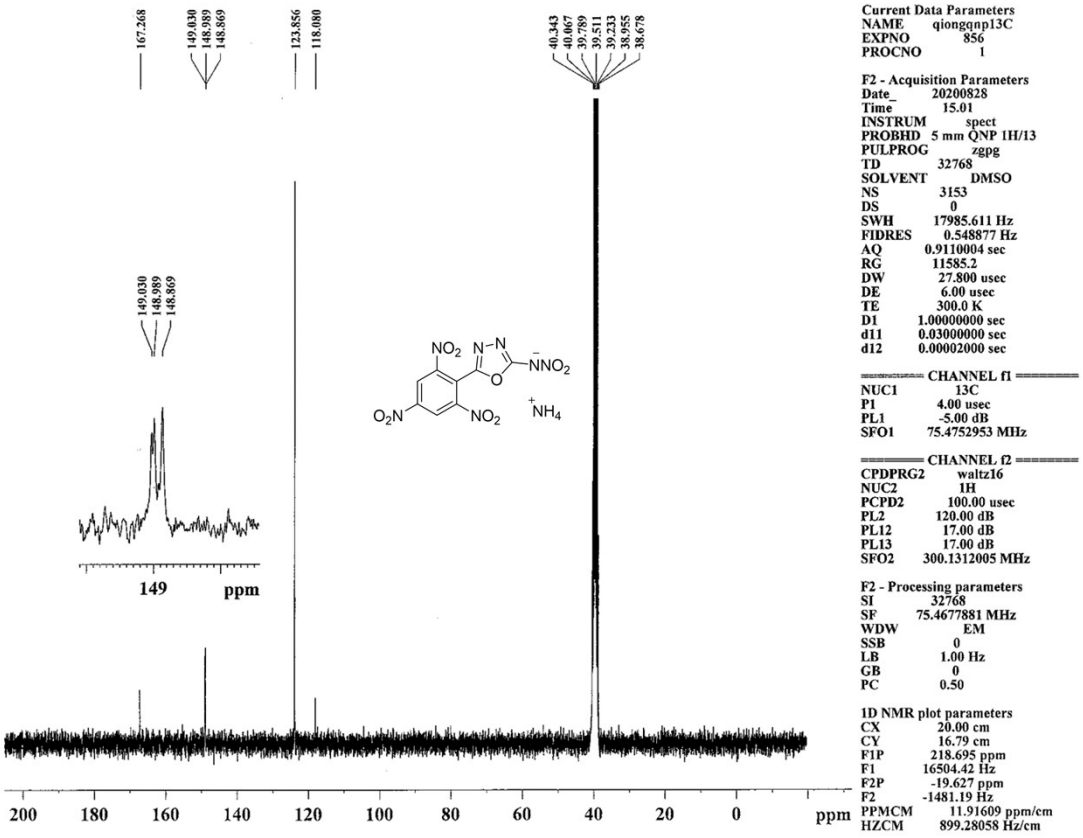


Figure S8 ^{13}C-NMR spectrum of **4** in d_6-DMSO.

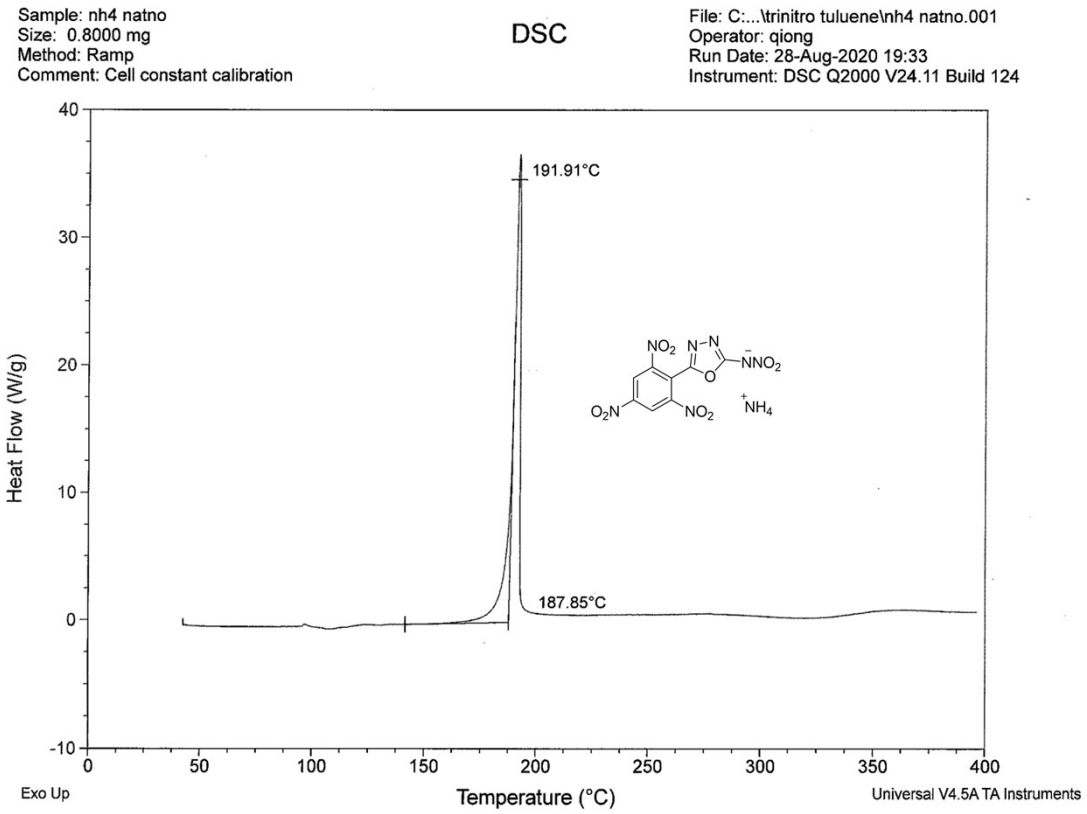


Figure S9 DSC plot of **4**.

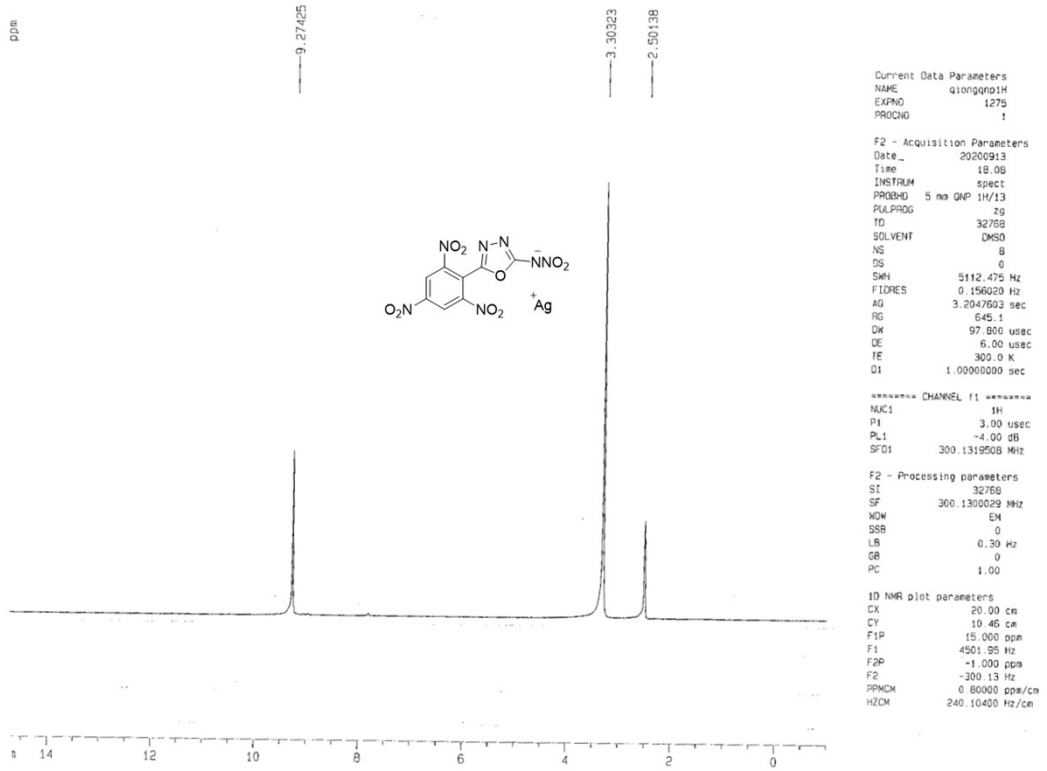


Figure S10 ^{1}H-NMR spectrum of **5** in d_6-DMSO.

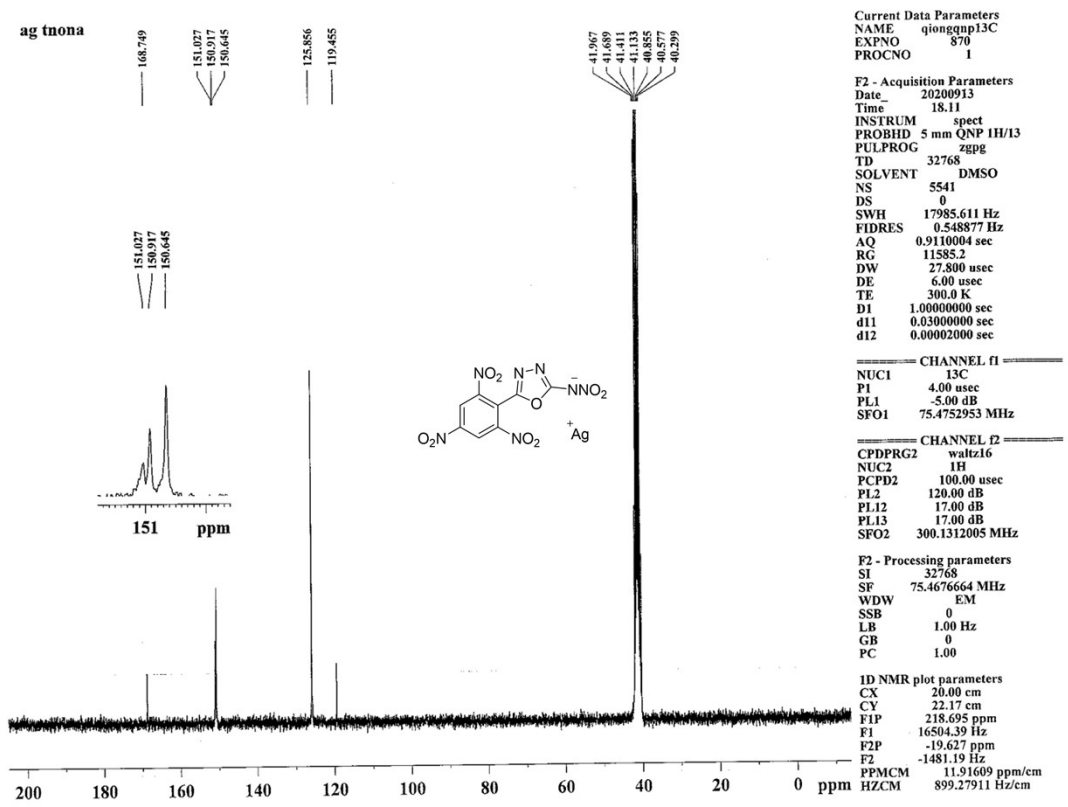


Figure S11 ^{13}C-NMR spectrum of **5** in d_6-DMSO.

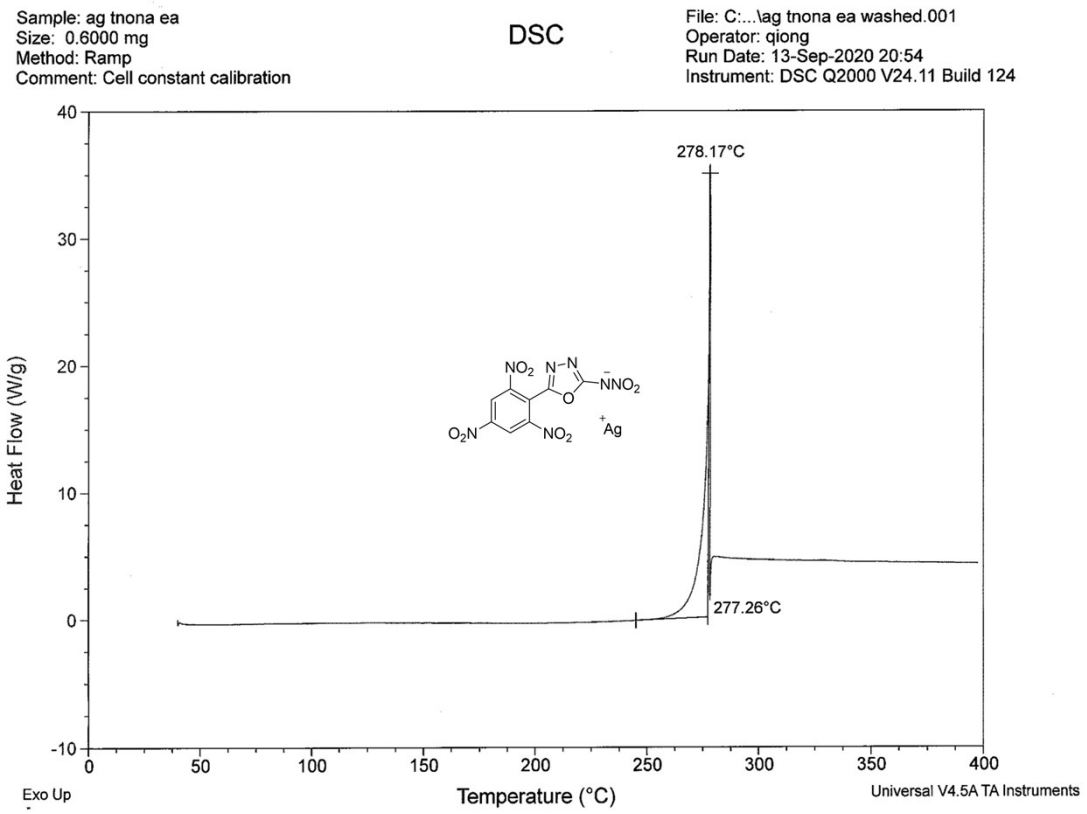


Figure S12 DSC plot of **5**.

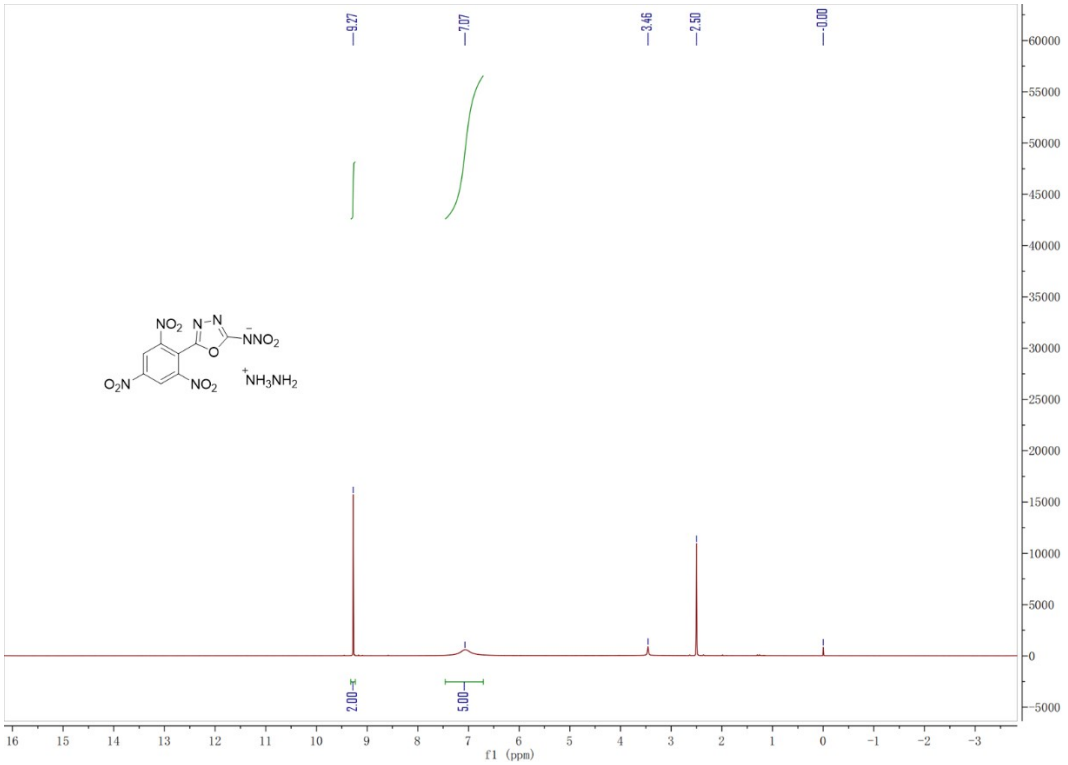


Figure S13 ^{1}H-NMR spectrum of **6a** in d_6-DMSO.

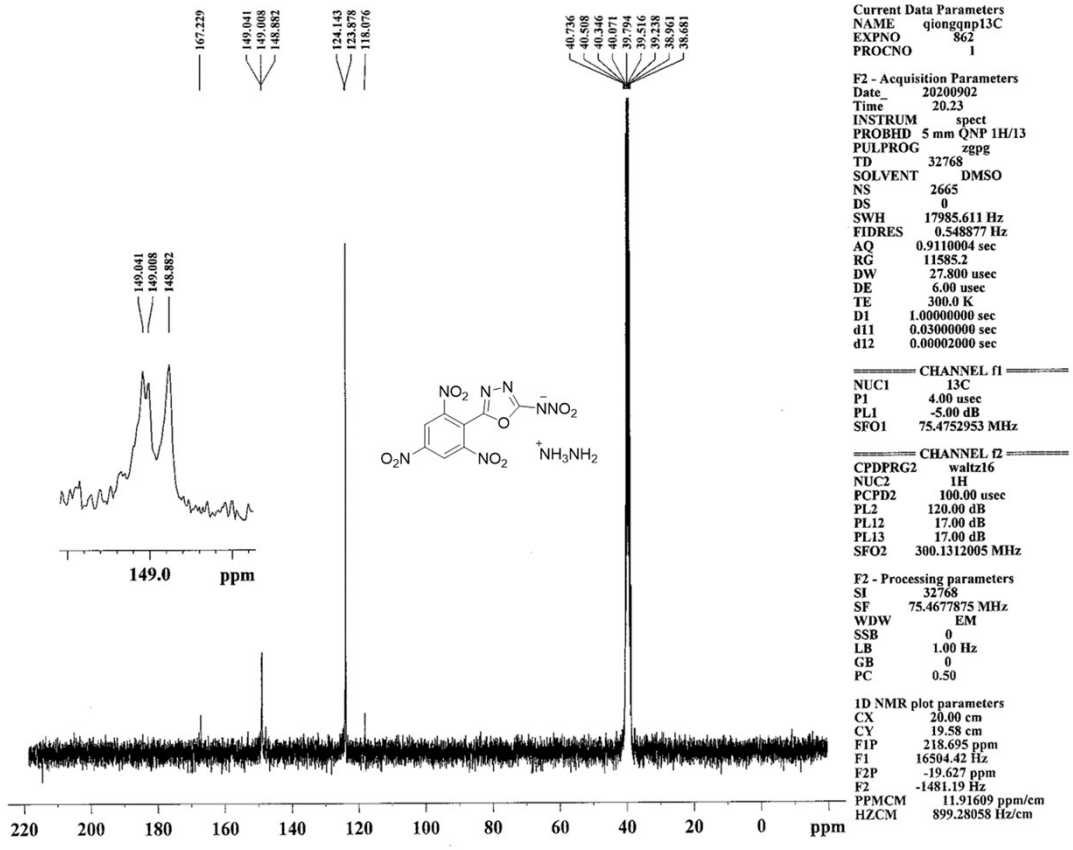


Figure S14 ^{13}C-NMR spectrum of **6a** in d_6-DMSO.

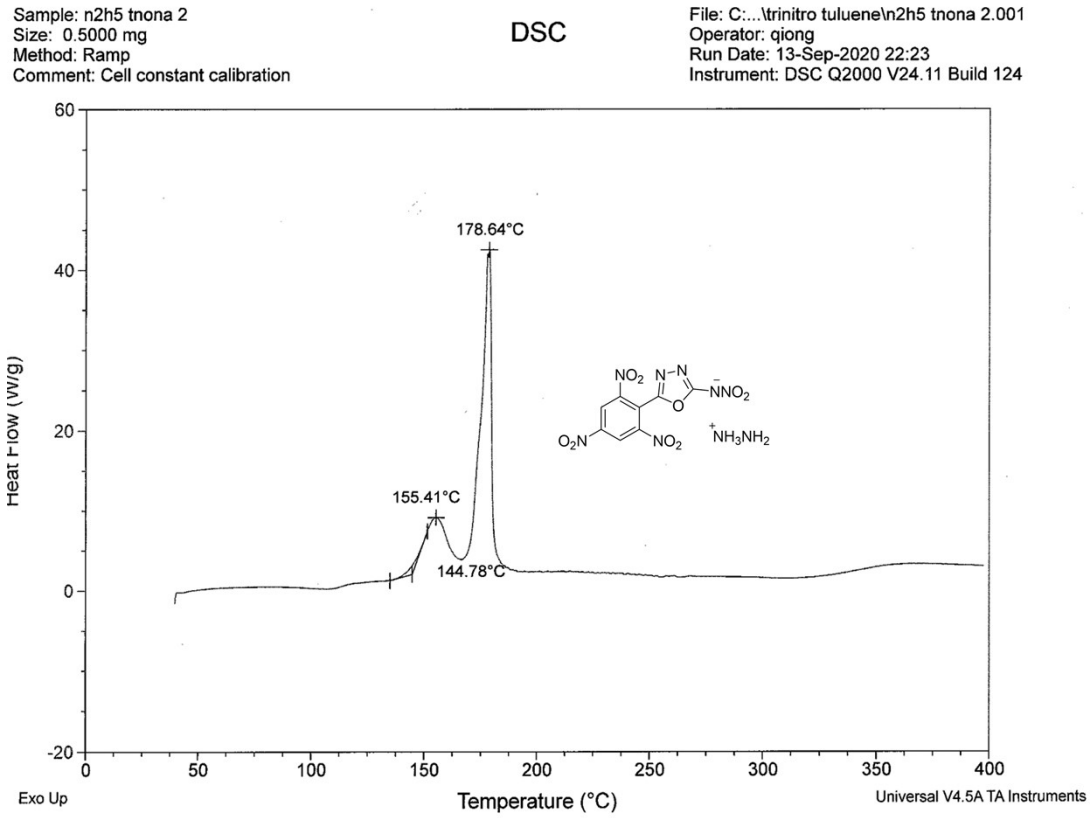


Figure S15 DSC plot of **6a**.

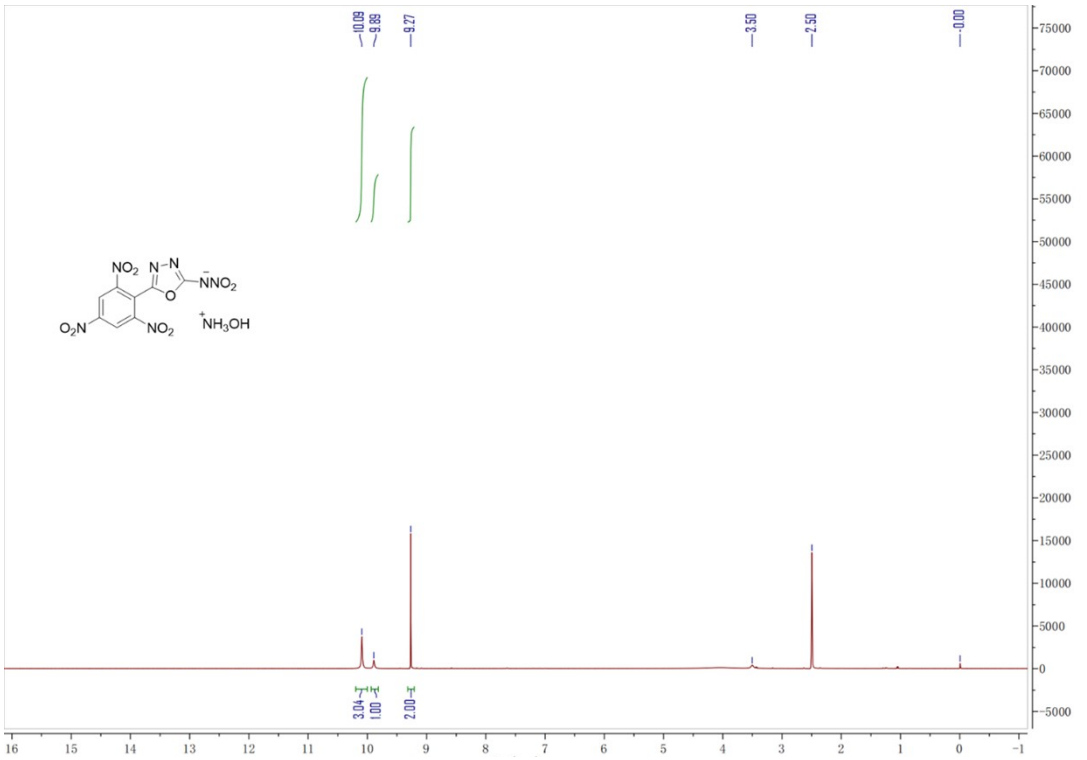


Figure S16 ^{1}H-NMR spectrum of **6b** in d_6-DMSO.

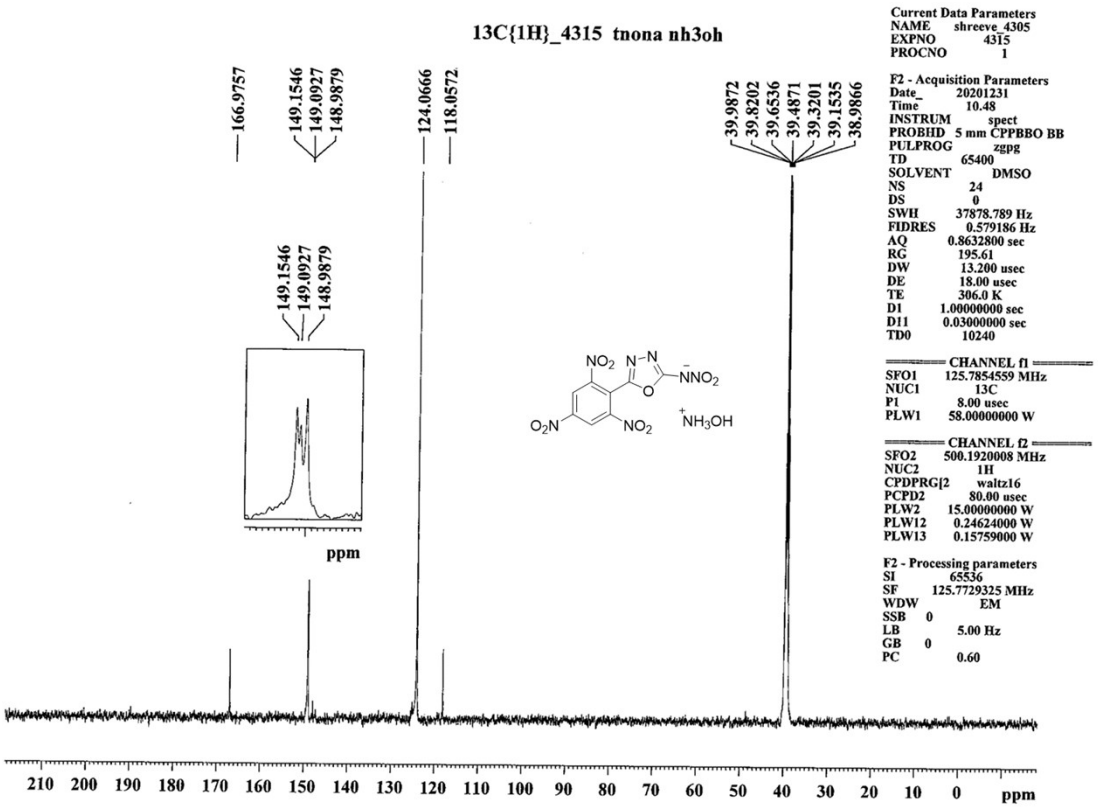


Figure S17 ^{13}C-NMR spectrum of **6b** in d_6-DMSO.

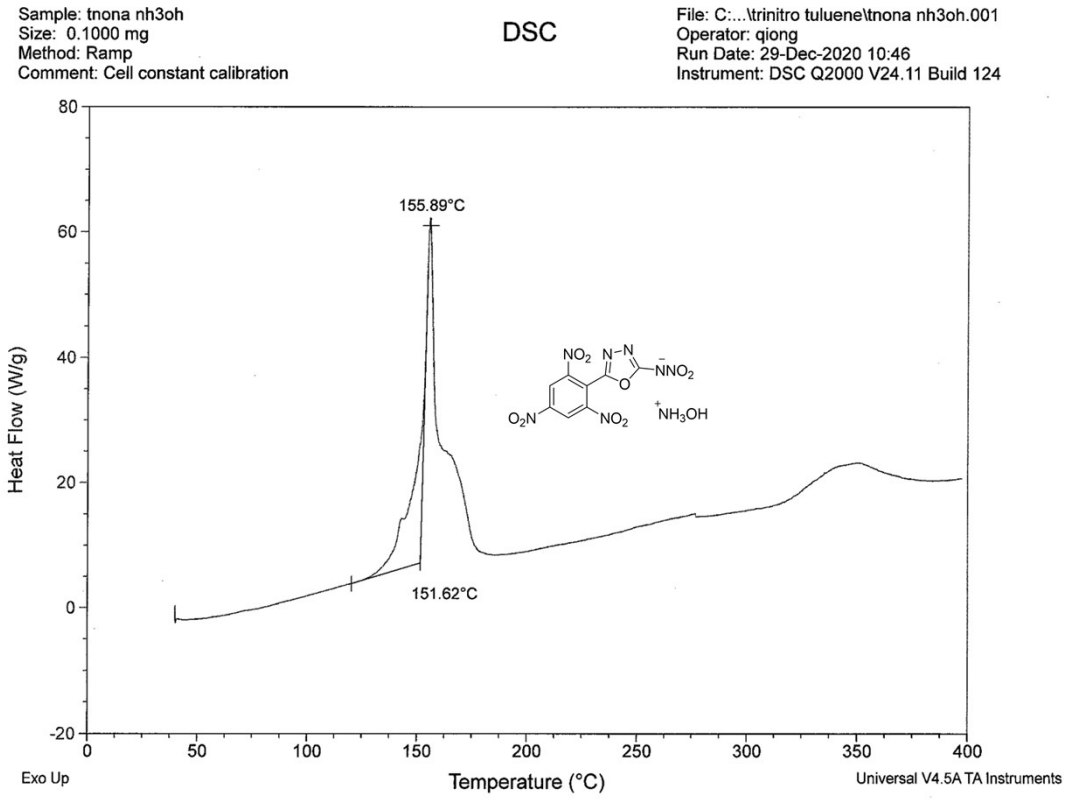


Figure S18 DSC plot of **6b**.

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